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FINAL REPORT

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Parallel Multi-Scale Algorithms and Applications to Combustion and Turbulence

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Abstract

In this project, the main objective was to develop multiresolution wavelet algorithm to study the flame acceleration and to understand the mechanism of the transition of deflagration to detonation. In the first half year of the project, The author completed the study of two dimensional detonation waves based on hybrid high order methods (a combination of high order Essentially Non-oscillatory (ENO) methods and spectral methods and Shock Tracking methods). The result on the detonation waves was published in the AIAA Journal. In the remaining time of the two years, first, the author completed the theoretical and algorithmic studies of the adaptive wavelet method, which could handle nonperiodic boundary conditions and nonlinear time dependent PDE's (The result was published in the SIAM Journal of Numerical Analysis). Secondly, the author implemented the adaptive wavelet methods for the solution of one-dimensional flame propagation; thirdly, the author developed a Fortran code WL2D (more than 13,000 lines) for the two dimensional multi-scale wavelet algorithms with an efficient data structure and implemented a second order implicit factorized scheme for the adaptive wavelet methods.

1 Hybrid High Order Methods for Detonation Waves

Partially supported by this grant, we completed the development of high order hybrid numerical simulation of two dimensional detonation waves. The major finding of this work was that the cellular structure of detonation waves depended very sensitively on the numerical dissipation of the algorithms representing detonation fronts. Further studies of the work in three dimensional cases were needed to understand the three dimensional effects of detonation waves. One paper summarizing the results of this study was published in AIAA Journal, Vol. 33, Number 3, pp 1248-1255.

2 Parallel Multi-scale Wavelet Algorithms

In an attempt to design multiscale methods for the study of deflagration to detonation transition (DDT) problem, we constructed a wavelet collocation multi-resolution algorithm for the initial value boundary problem of nonlinear PDE's. The key component in this collocation method was a so-called "Discrete Wavelet Transform" (DWT) which mapped a solution between the physical space and the wavelet coefficient space. The DWT transformation only took $O(N \log N)$ operations where N was the total number of unknowns. Therefore, the nonlinear term in the PDE could be easily treated in the physical space, and the derivatives of those nonlinear terms then computed in the wavelet space. The wavelet collocation methods had the following advantages: (a) the capability to handle arbitrary non-periodic boundary conditions; (b) the capability to treat general nonlinearity through the collocations of the PDE's; (c) flexibility of adaptive meshing in regions where high gradients of solution occur as in shock waves and turbulent premixed flames; (c) Capability of parallel and multi-grid implementations.

The following paragraph summarizes the key technical details of the algorithms. One paper containing some of the details of the results of this study was published in the Journal of *SIAM Numerical Analysis*, Volume 33, Number 3, pp. 937-970, June 1996.

2.1 Discrete Wavelet Transform (DWT)

The Discrete Wavelet Transformation (DWT) maps between a function at its sample points to the coefficients of its wavelet interpolation expansion. This transform in both direction will only take $O(N \log N)$, $N = 2^{(J+1)}L + L - 1$ operations for the $H^2(I)$ -wavelet basis.

Let $f(x)$ in $H_0^2(I)$, and we intend to construct a wavelet interpolation

$$\mathcal{P}_J f(x) \in V_0 \oplus W_0 \oplus W_1 \cdots \oplus W_J \text{ for } J \geq 0$$

First introduce two index spaces, for $W_j, j \geq 0$ we define

$$\mathcal{K}_j = \{-1, 0, \dots, n_j - 2\} \quad (1)$$

where $n_j = \dim W_j = 2^j L$ and for V_0 we define

$$\mathcal{K}_{-1} = \{-1, 0, \dots, L-3\} \quad (2)$$

Second, define the collocation points in domain $I = [0, L]$ associated with wavelet space $W_j, j \geq 0$ by

$$x_k^{(j)} = \frac{k + 1.5}{2^j}, \quad k \in \mathcal{K}_j \quad (3)$$

and for V_0 the collocation points are

$$x_k^{(-1)} = k + 2, \quad k \in \mathcal{K}_{-1} \quad (4)$$

The interpolation operator $\mathbf{I}_{V_0} f$ in V_0 interpolates $f(x)$ on collocation points $\{x_k^{(-1)}\}_{k \in \mathcal{K}_{-1}}$ while the interpolation operator $\mathbf{I}_{W_j} f$ in W_j interpolates any function $f(x)$ in $H_0^2(I)$ on collocation points $\{x_k^{(j)}\}_{k \in \mathcal{K}_j}$. The construction of the interpolant $\mathbf{I}_{W_j} f$ and $\mathbf{I}_{V_0} f$ involves the inversion of a tridiagonal matrix with size $\dim W_j = n_j$ or $\dim V_0 = L - 1$, respectively.

Now let us assume that the values of a function $f(x) \in H_0^2(I)$ are given on all the collocation points $\{x_k^{(j)}\}, k \in \mathcal{K}_j, -1 \leq j \leq J$, then the wavelet interpolation $\mathcal{P}_J f(x) \in V_0 \oplus W_0 \oplus W_1 \cdots \oplus W_J$ for $J \geq 0$ is defined as

$$\mathcal{P}_J f(x) = f_{-1}(x) + \sum_{j=0}^J f_j(x) \quad (5)$$

such that

$$\mathcal{P}_J f(x_k^{(j)}) = f(x_k^{(j)}), \quad \text{for } k \in \mathcal{K}_j, -1 \leq j \leq J$$

where

$$f_{-1}(x) = \mathbf{I}_{V_0} f(x) = \sum_{k \in \mathcal{K}_{-1}} \hat{f}_{-1,k} \phi_{0,k}(x) \in V_0$$

and for $j \geq 0$,

$$f_j(x) = \mathbf{I}_{W_j}(f^{(j)} - (\mathcal{P}_{j-1} f)^{(j)}) = \sum_{k \in \mathcal{K}_j} \hat{f}_{j,k} \psi_{j,k}(x) \in W_j. \quad (6)$$

Let us denote $\mathbf{f} = (f^{(-1)}, f^{(0)}, \dots, f^{(J)})^T$ the values of $f(x)$ on all interpolation points on all levels, $\mathbf{f}^{(j)} = \{f(x_k^{(j)})\}_{k \in \mathcal{K}_j}, j \geq -1$ and $\hat{\mathbf{f}} = (\hat{f}^{(-1)}, \hat{f}^{(0)}, \dots, \hat{f}^{(J)})^T$ the wavelet coefficients in the expansion (5), $\hat{\mathbf{f}}^{(j)} = \{\hat{f}_{j,k}\}_{k \in \mathcal{K}_j}, j \geq -1$.

A fast discrete wavelet transform (DWT) was proposed for an efficient transformation between point values \mathbf{f} and $\hat{\mathbf{f}}$ with operation counts of order $O(N \ln N)$ in both directions. The efficiency of the transformation is based on the fact that $\phi_{-1,k}(x), \psi_{j,k}(x), k \in \mathcal{K}_j$ form a hierarchical nodal basis on all levels of collocation points $\{x_k^{(j)}\}, -1 \leq j \leq J, k \in \mathcal{K}_j$.

2.2 Wavelet Collocation Methods for PDE's

We consider a collocation method based on the DWT transform for time dependent PDE's. Let $u = u(x, t)$ be the solution of the following initial boundary value problem

$$\begin{cases} u_t + f_x(u) = u_{xx} + g(u), x \in [0, L], t \geq 0 \\ u(0, t) = g_0(t) \\ Bu(L, t) = g_1(t) \\ Bu(x, 0) = f(x) \end{cases} \quad (7)$$

where B is the boundary condition operator which could be either Dirichlet boundary conditions or Neuman type or Robin type boundary conditions.

The numerical solution $u_J(x, t)$ will be represented by a unique decomposition in the cubic spline wavelet decomposition of $H^2(I) - V_0 \oplus W_0 \oplus \dots \oplus W_J, J \geq 0$, namely

$$u_J(x) = I_{b,J}u(x) + u_{-1}(x) + u_0(x) + \dots + u_J(x) \quad (8)$$

where cubic spline $I_{b,J}u(x, t)$ consists of the nonhomogeneity of $u(x, t)$ on both boundaries, and the coefficients $\hat{u}_{j,k}(t)$ are all functions of t . Using the DWT transform, we can also identify the numerical solution $u_J(x, t)$ by its point values on all collocation points, we put all these values in vector $\mathbf{u} = \mathbf{u}(t)$, i.e.

$$\mathbf{u} = \mathbf{u}(t) = (u^{(-1)}, u^{(0)}, \dots, u^{(J)})^T$$

where $\mathbf{u}^{(j)} = \{u(x_k^{(j)}, t)\}, k \in \mathcal{K}_j$ for $j \geq -1$.

To solve for the unknown solution vector $\mathbf{u}(t)$, we collocate the PDE (7) on all collocation points, then we have the following semi-discretized wavelet collocation method.

Semi-Discretized Wavelet Collocation Methods

$$\begin{cases} u_{Jt} + f_x(u_J) = u_{Jxx} + g(u_J)|_{x=x_k^{(j)}} \\ Bu_J(0, t) = g_0(t) \\ Bu_J(L, t) = g_1(t) \\ u_J(x_k^{(j)}, 0) = f(x_k^{(j)}) \end{cases} \quad (9)$$

where $k \in \mathcal{K}_j - 1 \leq j \leq J$.

Computation of $f_x(x_k^{(j)}) = f_x(u_J(x_k^{(j)}))$

Step 1 Given $\mathbf{u} = (u^{(-1)}, u^{(0)}, \dots, u^{(J)})^T$, compute $\mathbf{f}^{(j)} = \{f(u_k^{(j)})\}, k \in \mathcal{K}_j, j \geq -1$ and define

$$\mathbf{f} = (f^{(-1)}, f^{(0)}, \dots, f^{(J)})^T;$$

Step 2 Compute the wavelet interpolation expansion using DWT transform for \mathbf{f} as in (5)

Step 3 Differentiate the interpolation expansion and evaluate at all collocation points $x_k^{(j)}$,

which is taken as $f_x((x_k^{(j)})) = f_x(u_J(x_k^{(j)}))$.

The total cost of computing the derivatives will be $(5J + 12)N \leq 5N \log N$.

2.3 Adaptive Meshing

In equations (8), $u_J(x)$ is expressed using the full set of collocation points $\{x_k^{(j)}\}$. As most of the wavelet expansion coefficients $\hat{u}_{j,k}$ for large j can be ignored within a given tolerance ϵ . So we can dynamically adjust the number and locations of the collocation points used in the wavelet expansions, reducing significantly the cost of the scheme while providing enough resolution in the regions where the solution varies significantly.

Let $\epsilon \geq 0$ be a prescribed tolerance and $j \geq 0$, $\ell = \ell(\epsilon) = \min(\frac{n_j}{2}, -\log \epsilon / \log \alpha)$, $\alpha = 13.98$.

Step 1. First locate the range for the index k ,

$$(k'_1, l'_1), \dots, (k'_m, l'_m), m = m(j, \epsilon) \quad (10)$$

such that

$$|\hat{u}_{j,k}| \leq \epsilon, \quad k'_i \leq k \leq l'_i, \quad i = 1, \dots, m. \quad (11)$$

Step 2. Ignore $\hat{u}_{j,k}$ in (8) for $k_i \leq k \leq l_i, i = 1, \dots, m, k_i = k'_i + \ell + 3, l_i = l'_i - \ell - 3$, namely we redefine $u_j(x)$ as

$$u_j(x) := \sum_{k \in \mathcal{K}_j \setminus \mathcal{K}'_j} \hat{u}_{j,k} \psi_{j,k}(x)$$

where $\mathcal{K}'_j = \bigcup_{1 \leq i \leq m} [k_i, l_i]$.

Step 3. The new collocation points and unknowns will be

$$\{x_k^{(j)}\}, u_j(x_k^{(j)}), k \in \mathcal{K}_{-1} \text{ if } j = -1; k \in \mathcal{K}_j \setminus \mathcal{K}'_j \text{ if } j \geq 0.$$

2.4 Data Structure for Two Dimensional Adaptive Wavelet Algorithms

We have developed an efficient data structure for two and three dimensional wavelet approximations. Being an adaptive scheme in nature, an efficient data structure for handling numerical solutions in a wavelet framework is the first step in making a theoretical potential into real application. We have used sparse matrix data structure (compressed row and compressed column vector technique) in treating the data structure on each wavelet space $W_i^x \times W_j^y$ in the case of two dimensional approximations. Such approach have the advantage of only storing the mesh points used in the adaptive wavelet approximations and easy access to numerical data on each constant x and y lines for the numerical differentiations.

Data Structure - 1-D

One Dimensional Case:

$$u = \{u^{(-1)}, u^{(0)}, \dots, u^{(j)}, \dots, u^{(j)}\}$$

$$\in V_0 \oplus W_0 \oplus W_1 \oplus \dots \oplus W_J$$

$$u^{(j)} = \{u_k^{(j)}\}_{1 \leq k \leq n_j}$$

where n_j - number of mesh points on level W_j

[1] *pointer(j)* - pointer of first element of $u^{(j)}$

[2] *npts(j)* - number of elements in $u^{(j)} - n_j$

[3] *index(1 : n_j)* - collocation point location indices

Data Structure - 2-D

$$\sum_{j_x=-1}^J W_{j_x}^x \times \sum_{j_y=-1}^J W_{j_y}^y = \dots W_{j_x}^x \times W_{j_y}^y \dots$$

Mesh on level $(j_x, j_y) - W_{j_x}^x \times W_{j_y}^y$

- Compressed Row Form :

i-th row:

lenrow(*i*, *jx*, *jy*) - length of i-th row

ipr(*i*, *jx*, *jy*) - pointer of 1st mesh on i-th row

icn(:, *jx*, *jy*) - column indices of i-th row

- Compressed column Form :

i-th column:

lencol(*i*, *jx*, *jy*) - length of i-th row

ipc(*i*, *jx*, *jy*) - pointer of 1st mesh on i-th row

irn(:, *jx*, *jy*) - column indices of i-th row

2.5 Fast Time Integration - Factorized ADI Wavelet Approach

On the issue of time integration, we have successfully implemented a second order implicit factorized scheme of Beam and Warming type for the adaptive wavelet methods. Unlike many other adaptive methods (finite element and finite difference), the adaptive wavelet methods actually can be easily implemented using an ADI approach. So, solution of the algebraic systems from the implicit discretization of 2-dimensional diffusion operators is replaced by that of only 1-dimensional operators, thus speeding up the time integrations tremendously.

Example: Beam Warming schemes for Euler Equations.

$$\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} + \frac{\partial G(u)}{\partial y} = 0$$

$$(I + \frac{\Delta t}{2} D_x A^n)(I + \frac{\Delta t}{2} D_y B^n) u^{n+1}$$

$$= (I - \frac{\Delta t}{2} D_x A^n)(I - \frac{\Delta t}{2} D_y B^n) u^n$$

D_x and D_y the wavelet derivatives.

3 Computational Results of Multi-scale Wavelet Algorithms for 2-D flames

We have developed a two dimensional code WL2D based on the adaptive wavelet approximations. The following eight pages summarize the simulation results of two dimensional cellular and planar flame propagations.

[1] Two Dimensional Perturbed Cellular Flame

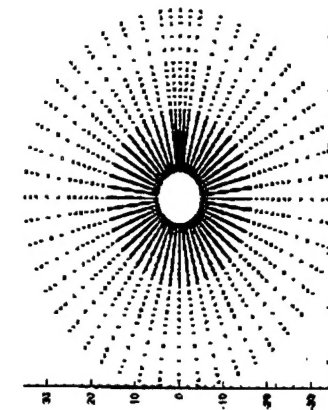
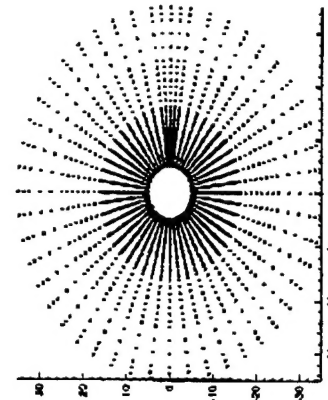
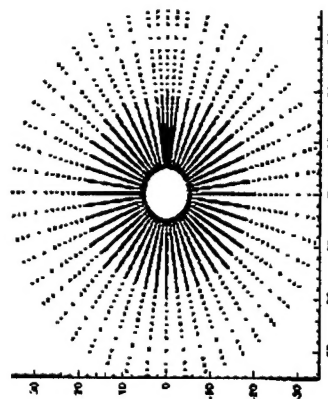
$$\begin{aligned}\Theta_t &= \Delta \Theta - \kappa \frac{\Theta_r}{r} + \Omega \\ C_t &= \frac{\Delta C}{L} - \kappa \frac{C_r}{r} - \Omega\end{aligned}$$

where Δ is the Laplace Operator Initial Condition:

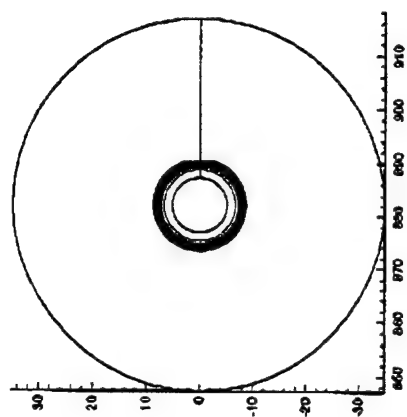
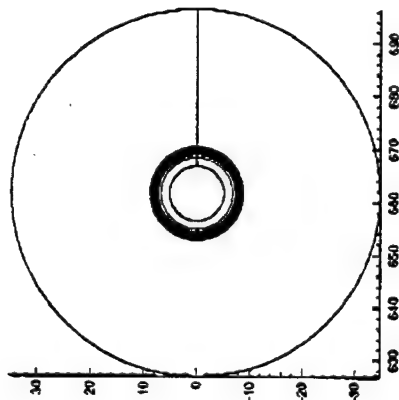
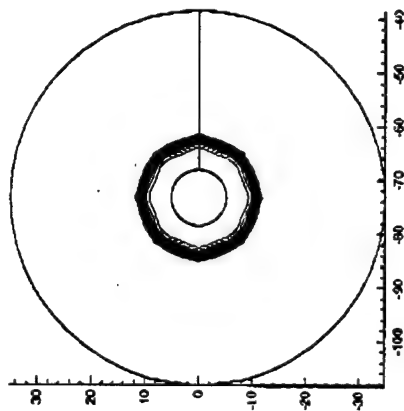
$$\begin{aligned}\Theta &= \left(\frac{r}{\kappa}\right)^\kappa + O\left(\frac{1}{M}\right) \\ C &= (1 - \Theta) + O\left(\frac{1}{M}\right)\end{aligned}$$

+ perturbation of flame fronts

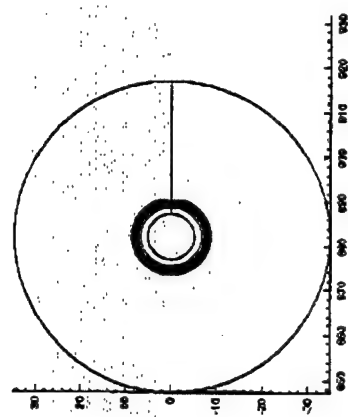
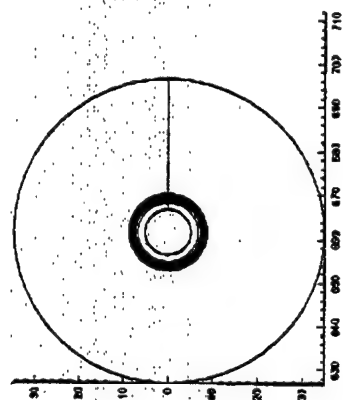
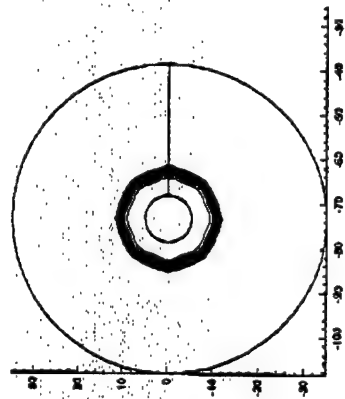
$T=0, N=2967; T=10, N=2749; T=13, N=2791$



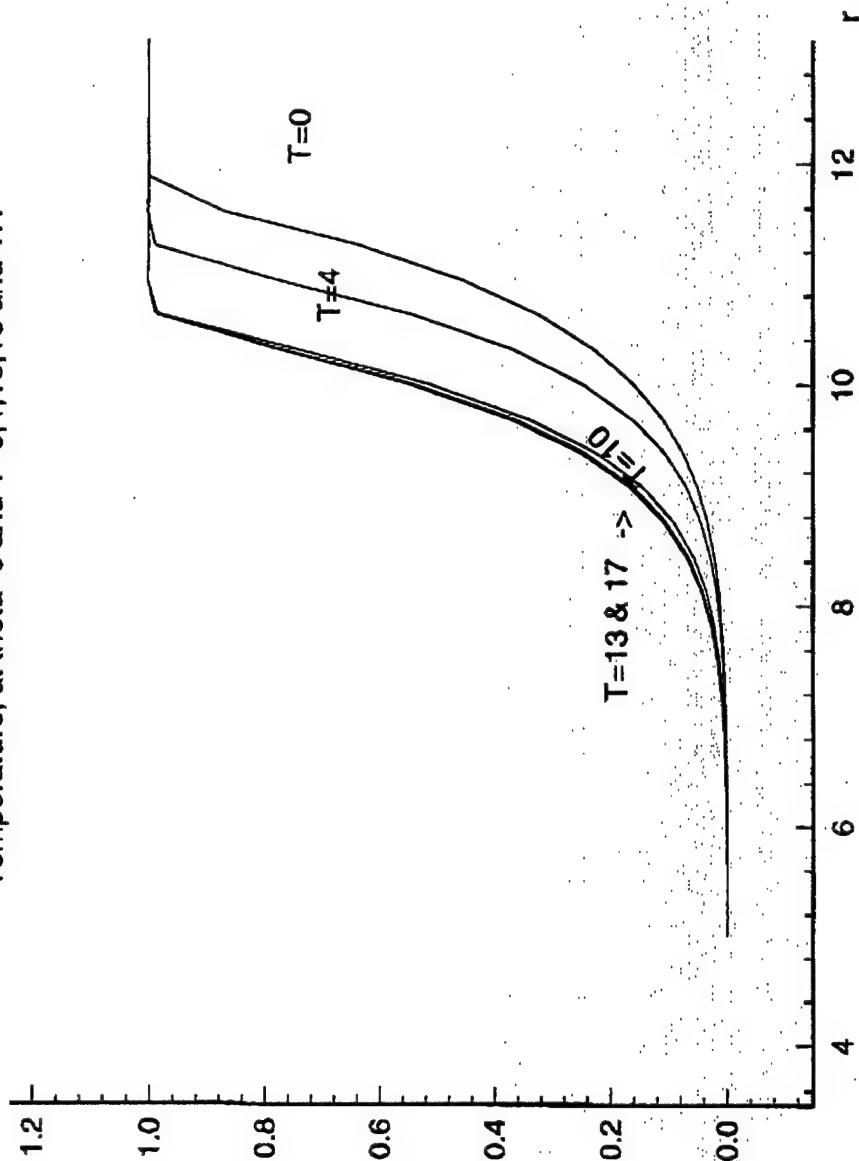
$T=0, 10, 13$, Reactant Mass Fraction



$T=0, 10, 13$, Temperature



Temperature, at $\theta=0$ and $T=0, 4, 10, 13$ and 17 .



[2] Two dimensional Perturbed planar flames

$$\Theta_t = \Delta \Theta + \Omega$$

$$C_t = \frac{\Delta C}{L} - \Omega$$

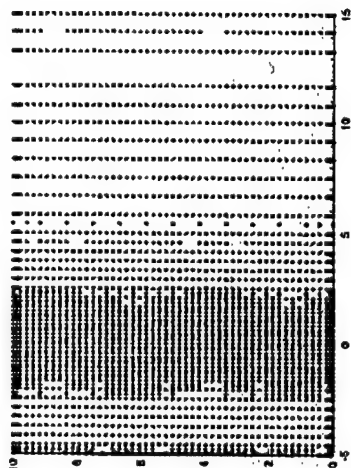
where Δ is the Laplace Operator Initial Condition:

$$\Theta = \exp x \text{ if } x \leq 0$$

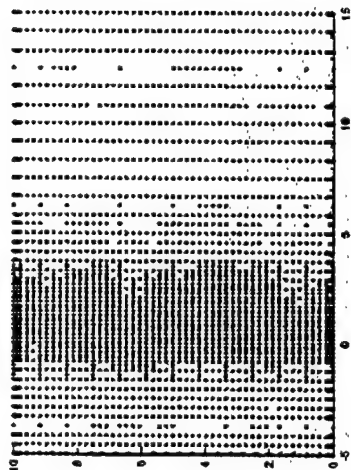
$$= 1 \text{ if } x > 0$$

$$C = 1 - \Theta$$

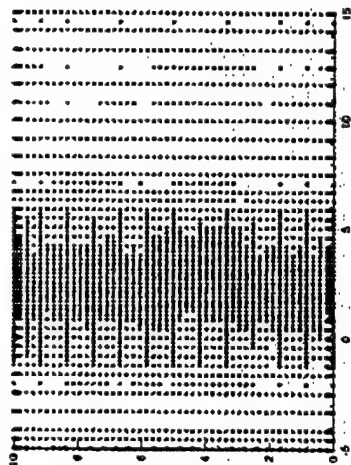
$T=0, N=2438$



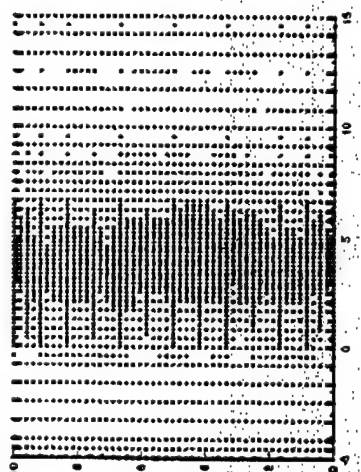
$T=1, N=2393$



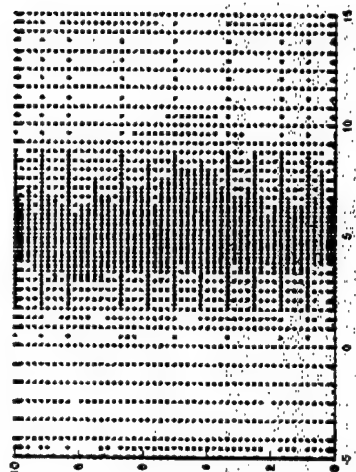
$T=2, N=2419$



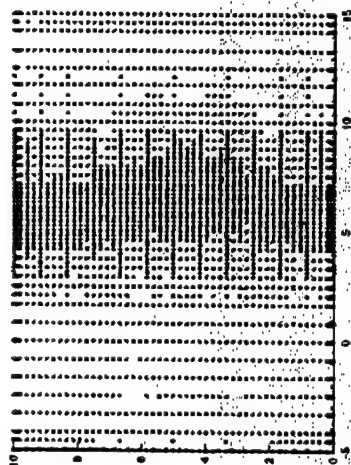
$T=3, N=2400$



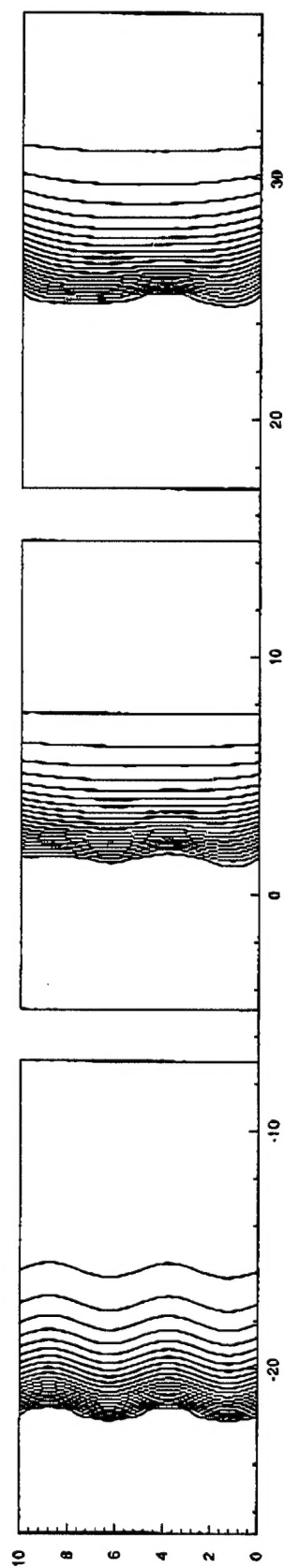
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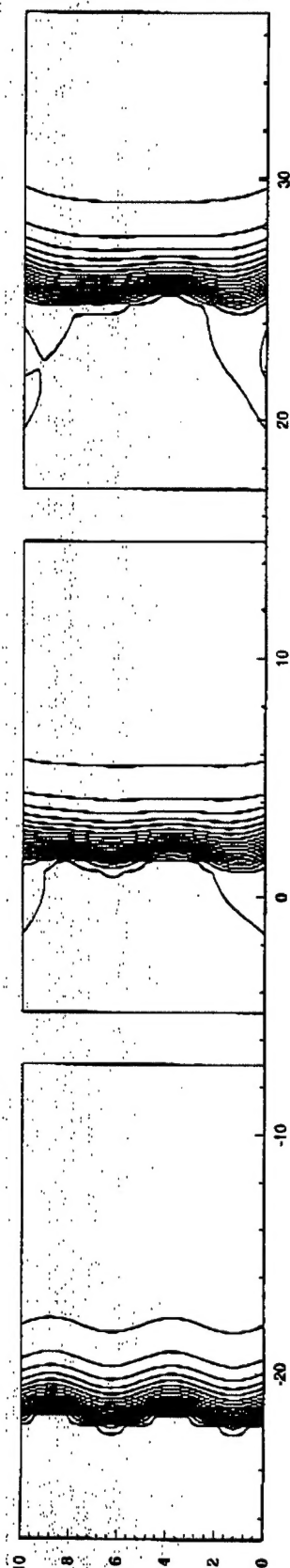
$T=5, N=2403$



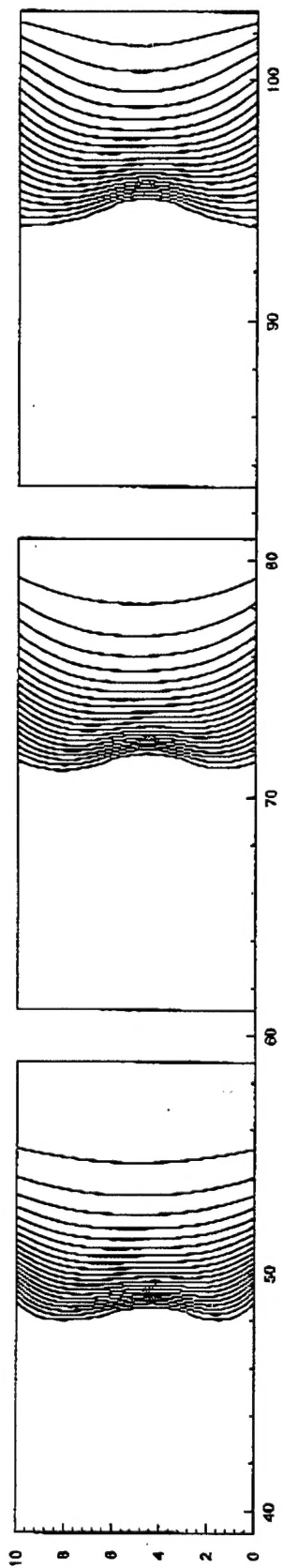
$T = 0, 1, 2$, Reactant Mass Fraction



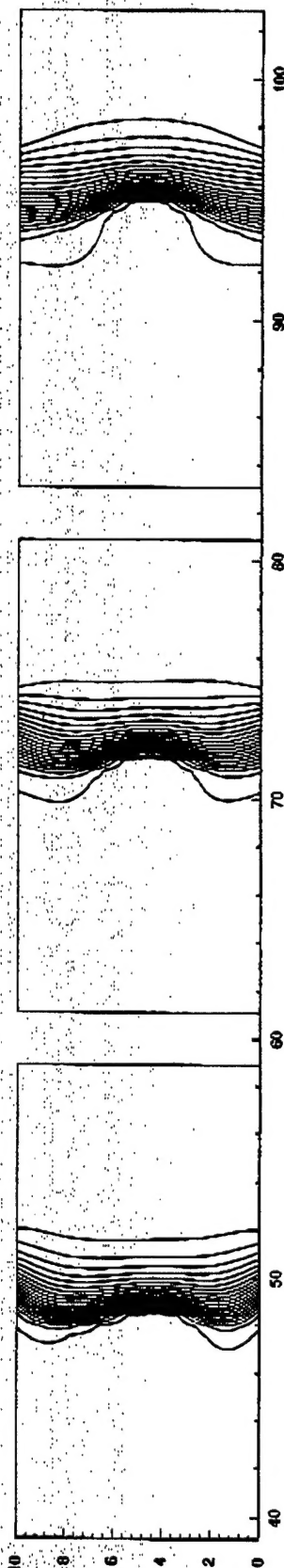
$T = 0, 1, 2$, Temperature



$T = 3, 4, 5$ Reactant Mass Fraction



$T = 3, 4, 5$ temperature



4 Publications

The following publications are supported by the AFOSR grant # F49620-94-1-0317

Appeared

[1] High-order Hybrid Numerical Simulations of Two Dimensional Detonation Waves, AIAA J. Vol. 33, No. 7, pp 1248-1255, (July, 1995).

[2] Direct numerical calculation of neutral stability curve for one dimensional detonations, (with W.H. Oh, Y.L. Zhu), *SIAM J. Scientific Computing* Vol. 17, No. 4, pp. 814-829, July, 1996.

[3] Adaptive Wavelet Collocation Method for the Initial Value Boundary Problem of Nonlinear PDE's, (with J.Z. Wang), *SIAM Numerical Analysis*, Volume 33, Number 3, June 1996.

Submitted

[1] A fast wavelet collocation method for high speed circuit simulation (with Dian Zhou), submitted to IEEE transaction on circuits and systems, May, 1996.

[2] An adaptive wavelet method for nonlinear circuit simulation (with Dian Zhou and W, Zhang) submitted to IEEE transaction on CAD, May, 1996.

5 Personnel Supported

Wei Cai, PI

6 Appendix: 2-D wavelet Computer Code WL2D